

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042467.D
 Acq On : 23 Jul 2024 13:25
 Operator : JC/MD
 Sample : VX0724WBL01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK691

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042467.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	21	25	34	rBV	61132	74428	8.21%	1.105%
2	1.367	43	46	58	rBV	76963	97824	10.80%	1.452%
3	1.642	88	91	100	rVB	50385	67547	7.46%	1.003%
4	2.294	192	198	212	rBV	146871	240241	26.52%	3.566%
5	2.666	257	259	261	rVB2	254	194	0.02%	0.003%
6	2.703	261	265	266	rBV2	310	332	0.04%	0.005%
7	2.782	274	278	287	rBV3	1550	3003	0.33%	0.045%
8	2.946	298	305	313	rVB3	911	2131	0.24%	0.032%
9	3.062	322	324	325	rBV	158	131	0.01%	0.002%
10	3.081	325	327	330	rVV2	206	260	0.03%	0.004%
11	3.142	336	337	339	rBV2	170	156	0.02%	0.002%
12	3.184	342	344	345	rVV	184	127	0.01%	0.002%
13	3.203	345	347	350	rVV	134	113	0.01%	0.002%
14	3.422	380	383	384	rVB2	136	121	0.01%	0.002%
15	3.495	392	395	397	rBV2	109	139	0.02%	0.002%
16	3.922	461	465	468	rVB	230	233	0.03%	0.003%
17	3.977	470	474	476	rBV2	136	162	0.02%	0.002%
18	4.026	479	482	485	rBV2	139	180	0.02%	0.003%
19	4.190	505	509	511	rVB2	168	178	0.02%	0.003%
20	4.336	531	533	538	rVB2	132	159	0.02%	0.002%
21	4.464	547	554	583	rBV	69850	215015	23.73%	3.191%
22	4.879	620	622	623	rBV2	265	215	0.02%	0.003%
23	4.940	630	632	634	rBV	194	129	0.01%	0.002%
24	5.056	636	651	669	rBV	113003	352449	38.90%	5.231%
25	5.397	699	707	712	rBV3	1559	4083	0.45%	0.061%
26	5.556	724	733	745	rBV4	1750	5899	0.65%	0.088%
27	5.641	745	747	751	rVB	148	134	0.01%	0.002%
28	5.684	751	754	756	rBV2	139	158	0.02%	0.002%
29	5.964	789	800	823	rBV2	306939	906041	100.00%	13.447%
30	6.275	848	851	852	rBV2	166	188	0.02%	0.003%
31	6.360	862	865	868	rBV	125	149	0.02%	0.002%
32	6.470	881	883	885	rBV	211	195	0.02%	0.003%
33	6.525	887	892	893	rVB2	131	174	0.02%	0.003%
34	6.549	893	896	899	rBV2	174	222	0.02%	0.003%
35	6.610	904	906	909	rBV2	125	130	0.01%	0.002%
36	6.763	921	931	947	rBV	220201	531032	58.61%	7.881%

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Integrator: RTE

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Title : VOC Analysis

37	7.116	983	989	1000	rVB5	1942	4579	0.51%	0.068%
38	7.220	1000	1006	1007	rBV3	301	395	0.04%	0.006%
39	7.312	1012	1021	1041	rBV	180445	407965	45.03%	6.055%
40	7.720	1086	1088	1091	rVB	211	208	0.02%	0.003%
41	7.958	1124	1127	1134	rBV3	586	1342	0.15%	0.020%
42	8.128	1152	1155	1156	rVB2	124	117	0.01%	0.002%
43	8.208	1166	1168	1171	rBV	183	109	0.01%	0.002%
44	8.324	1181	1187	1202	rVV	109865	187297	20.67%	2.780%
45	8.506	1215	1217	1218	rBV	401	302	0.03%	0.004%
46	8.592	1230	1231	1234	rBV	163	153	0.02%	0.002%
47	8.647	1234	1240	1252	rBV	463698	730530	80.63%	10.842%
48	8.951	1285	1290	1300	rBV	81215	121286	13.39%	1.800%
49	9.122	1316	1318	1319	rBV2	214	136	0.02%	0.002%
50	9.220	1333	1334	1337	rVB2	180	136	0.02%	0.002%
51	9.275	1339	1343	1351	rVB	8921	13162	1.45%	0.195%
52	9.384	1356	1361	1382	rBV	302431	468259	51.68%	6.950%
53	9.701	1410	1413	1416	rBV3	215	284	0.03%	0.004%
54	9.768	1422	1424	1425	rBV	238	148	0.02%	0.002%
55	9.848	1435	1437	1439	rVB2	168	135	0.01%	0.002%
56	10.055	1465	1471	1483	rBV	452425	615732	67.96%	9.139%
57	10.305	1508	1512	1519	rBV3	548	1102	0.12%	0.016%
58	10.488	1541	1542	1545	rVB	198	117	0.01%	0.002%
59	10.543	1550	1551	1555	rVB	165	135	0.01%	0.002%
60	10.573	1555	1556	1560	rBV	137	158	0.02%	0.002%
61	10.640	1565	1567	1568	rBV	298	225	0.02%	0.003%
62	10.841	1599	1600	1605	rVB	144	167	0.02%	0.002%
63	10.908	1609	1611	1614	rVB	157	150	0.02%	0.002%
64	10.963	1618	1620	1623	rVV2	314	298	0.03%	0.004%
65	11.097	1639	1642	1644	rVB3	325	389	0.04%	0.006%
66	11.189	1652	1657	1666	rBV	363652	477572	52.71%	7.088%
67	11.341	1680	1682	1684	rBV	312	217	0.02%	0.003%
68	11.366	1684	1686	1691	rVV2	187	248	0.03%	0.004%
69	11.457	1698	1701	1706	rVV4	338	497	0.05%	0.007%
70	11.670	1733	1736	1738	rBV2	119	129	0.01%	0.002%
71	11.701	1740	1741	1744	rVB	178	123	0.01%	0.002%
72	11.866	1766	1768	1770	rBV	202	161	0.02%	0.002%
73	11.939	1777	1780	1782	rBV	170	148	0.02%	0.002%
74	11.975	1782	1786	1788	rBV3	642	912	0.10%	0.014%
75	12.024	1788	1794	1806	rBV	433351	550877	60.80%	8.176%
76	12.317	1837	1842	1852	rBV	482151	638444	70.47%	9.476%

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Integrator: RTE

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Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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 Title : VOC Analysis

77	12.530	1876	1877	1879	rBV	193	164	0.02%	0.002%
78	12.762	1912	1915	1918	rBV2	537	741	0.08%	0.011%
79	12.792	1918	1920	1925	rVV2	151	225	0.02%	0.003%
80	12.853	1929	1930	1933	rVB2	144	138	0.02%	0.002%
81	12.884	1933	1935	1937	rBV2	173	163	0.02%	0.002%
82	12.920	1939	1941	1944	rBV2	125	134	0.01%	0.002%
83	13.036	1958	1960	1963	rVB2	119	114	0.01%	0.002%
84	13.115	1970	1973	1978	rVB2	659	700	0.08%	0.010%
85	13.274	1997	1999	2001	rBV2	128	122	0.01%	0.002%
86	13.323	2005	2007	2010	rVB2	150	158	0.02%	0.002%
87	13.512	2035	2038	2041	rBV	139	170	0.02%	0.003%
88	13.548	2041	2044	2046	rBV2	113	132	0.01%	0.002%
89	13.597	2049	2052	2055	rBV3	869	1023	0.11%	0.015%
90	13.780	2079	2082	2087	rBV2	558	829	0.09%	0.012%
91	13.969	2109	2113	2115	rBV2	676	864	0.10%	0.013%
92	14.030	2122	2123	2125	rBV2	152	142	0.02%	0.002%
93	14.127	2134	2139	2143	rBV	1409	1995	0.22%	0.030%
94	14.164	2143	2145	2146	rBV	214	123	0.01%	0.002%
95	14.365	2177	2178	2182	rBV2	211	194	0.02%	0.003%
96	14.396	2182	2183	2185	rVB2	249	115	0.01%	0.002%
97	14.414	2185	2186	2190	rBV3	188	266	0.03%	0.004%
98	15.024	2284	2286	2287	rVB	326	164	0.02%	0.002%
99	15.359	2339	2341	2342	rBV	579	445	0.05%	0.007%
100	15.914	2430	2432	2433	rBV	543	374	0.04%	0.006%

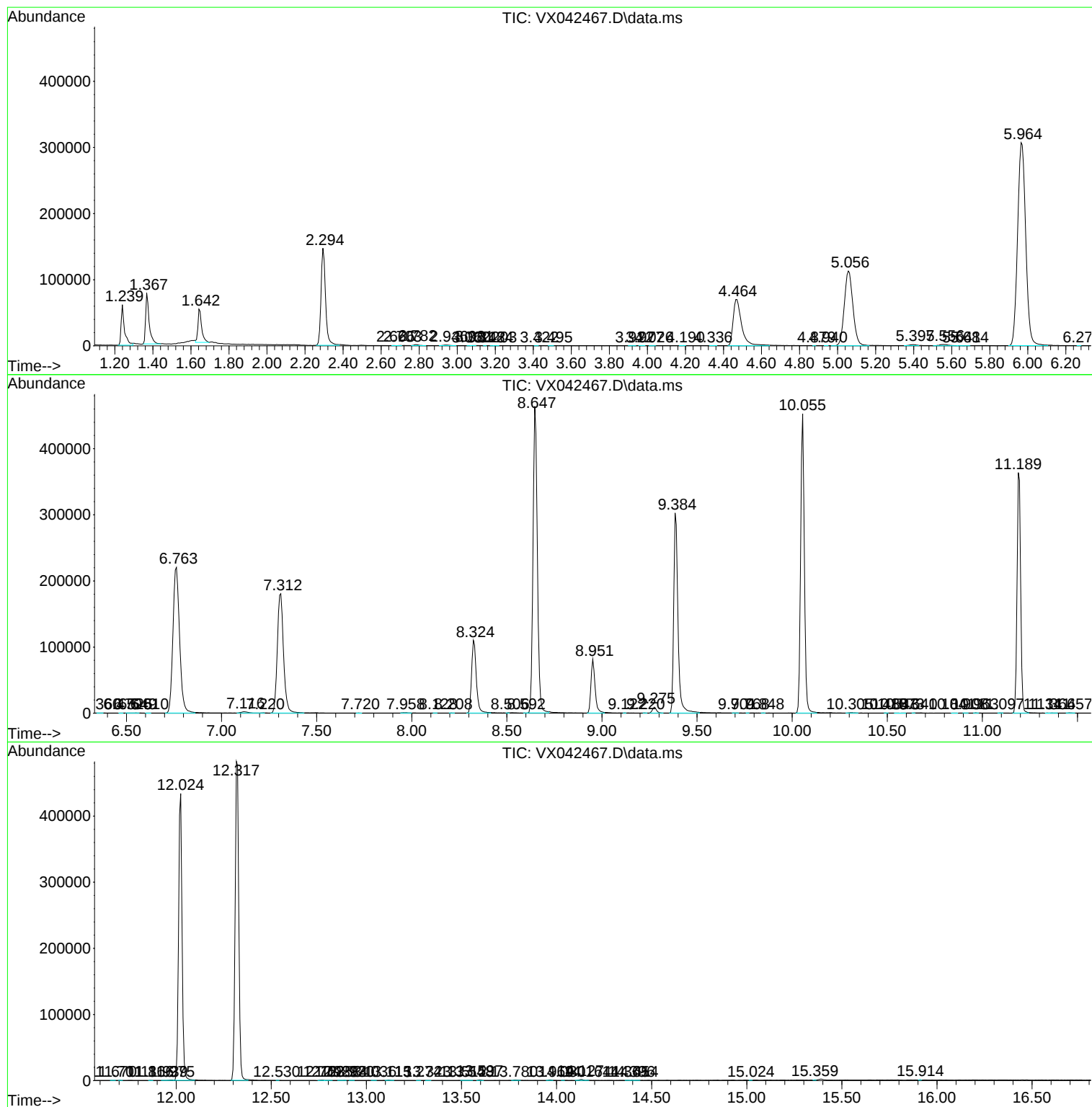
Sum of corrected areas: 6737711

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Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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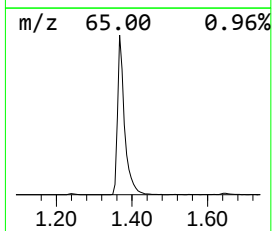
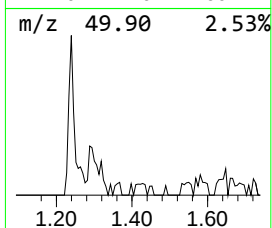
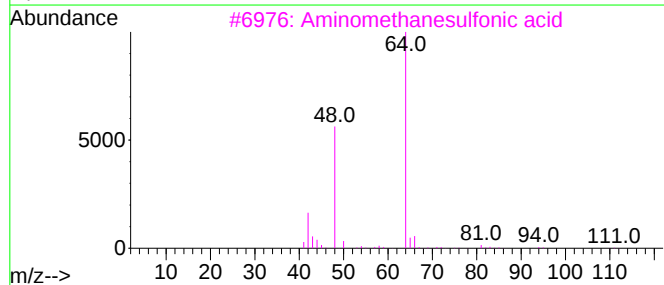
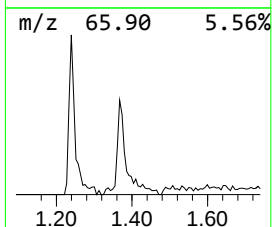
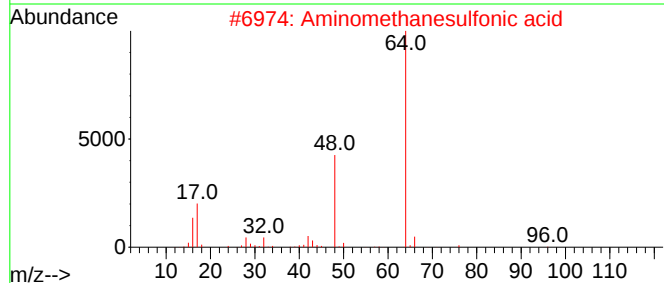
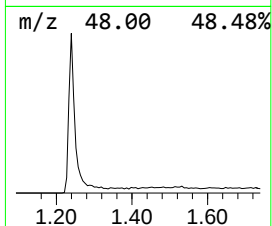
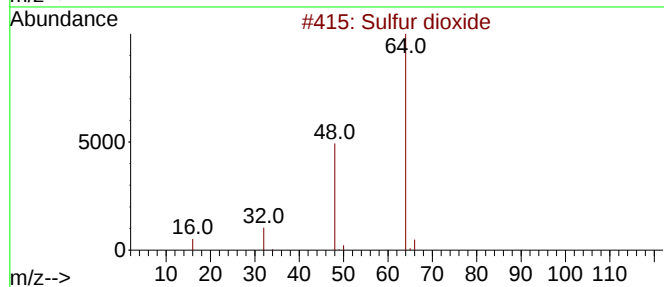
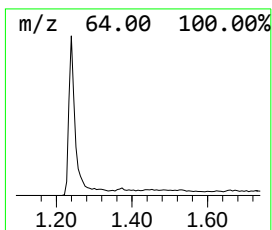
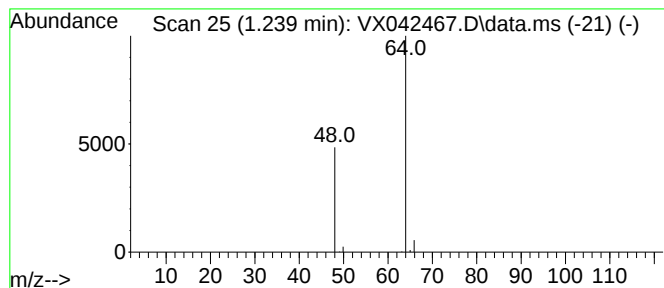
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	7.01 ug/L	74428	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.239	7.0	ug/L	74428	1	6.763	531032	50.0